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Origin of electron disproportionation in metallic sodium cobaltates

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Abstract

© 2016 American Physical Society.Recently, an unusual metallic state with a substantially nonuniform distribution of the charge and magnetic density in CoO2 planes was found experimentally in the NaxCoO2 compound with x>0.6. We have investigated the origin of such an electron disproportionation in the lamellar sodium cobaltates by calculating the ion states as a function of the strength of the electron correlations in the d(Co) shells within the GGA+U approximation for a system with a realistic crystal structure. It was found that the nonuniformity of spin and charge densities are induced by an ordering of the sodium cations and enhanced correlations. Two important magnetic states of cobalt lattice competing with each other at realistic values of the correlation parameter were found - low-spin hexagons lattice (LS) and higher-spin kagome lattice (HS-KSL). In the heterogeneous metallic HS-KSL phase, magnetic Co ions form a kagome structure. In LS phase, the kagome pattern is decomposed into hexagons and the Co ions possess the minimal values of their spin. Coexistence of these states could explain the emergence of the disproportionation with the peculiar kagome structure experimentally revealed in previous studies of the cobaltates.

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